

NASA TECHNICAL NOTE



NASA TN D-5879

C.1

LOAN COPY: RETURN
AFWL (WLOL)
KIRTLAND AFB, N

0132652



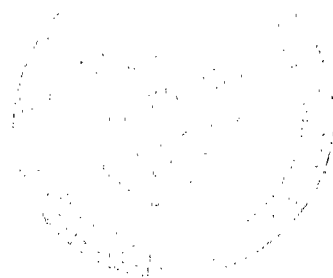
TECH LIBRARY KAFB, NM

A SYSTEMATIC METHOD OF CALCULATING REDUCED MATRIX ELEMENTS OF SINGLE-PARTICLE OPERATORS

by William F. Ford and Richard C. Braley

Lewis Research Center

Cleveland, Ohio 44135





0132652

1. Report No. NASA TN D-5879	2. Government Accession No.	3. Recipient's Catalog No.	
4. Title and Subtitle A SYSTEMATIC METHOD OF CALCULATING REDUCED MATRIX ELEMENTS OF SINGLE-PARTICLE OPERATORS		5. Report Date July 1970	
		6. Performing Organization Code	
7. Author(s) William F. Ford and Richard C. Braley		8. Performing Organization Report No. E-5366	
9. Performing Organization Name and Address Lewis Research Center National Aeronautics and Space Administration Cleveland, Ohio 44135		10. Work Unit No. 129-02	
		11. Contract or Grant No.	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Washington, D. C. 20546		13. Type of Report and Period Covered Technical Note	
		14. Sponsoring Agency Code	
15. Supplementary Notes			
16. Abstract A great many nuclear properties involve the evaluation of reduced matrix elements of single-particle operators between the initial and final nuclear states. We have developed a systematic means of calculating such matrix elements in terms of the inelastic transition densities $\rho_{LSJ}^{if}(r)$, which essentially give the probability for absorption of angular momentum $J = L + S$ by the last nucleon as a function of its distance from the nuclear origin. These densities may be expanded in terms of Gauss-Laguerre functions, thus permitting substantial simplification in the matrix element calculation. A number of examples and useful formulas are presented.			
17. Key Words (Suggested by Author(s)) Nuclear reactions; Nuclear structure; Matrix elements of single-particle operators; Single-particle matrix elements		18. Distribution Statement Unclassified - unlimited	
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No. of Pages 34	22. Price* \$3.00

A SYSTEMATIC METHOD OF CALCULATING REDUCED MATRIX ELEMENTS OF SINGLE-PARTICLE OPERATORS

by William F. Ford and Richard C. Braley

Lewis Research Center

SUMMARY

The necessary mathematical apparatus for the evaluation of reduced matrix elements of single-particle operators is introduced and developed, and the matrix elements are expressed as sums of integrals over the inelastic transition densities $\rho_{LSJ}^{if}(r)$. A biorthogonal set of functions called Gauss-Laguerre functions is then defined, in terms of which the densities are expanded. The reduced matrix elements are reexpressed as sums involving the coefficients ρ_{LSJn}^{if} of the transition density expansion. A number of simple applications to static and dynamic nuclear properties is presented, and the more complicated case of nucleon scattering form factors is treated in detail. Various practical considerations related to the method are discussed and analyzed. Appendixes are devoted to the effects of distributed nuclear charge, the Coulomb form factor, and numerical examples for neon-20 (^{20}Ne) intended to serve as a test case for programs based on this method.

INTRODUCTION

Recent developments in the theory of nuclear structure have made it possible to describe collective vibrational or rotational nuclear modes in terms of the motion of the individual nucleons. This opens the way to more rigorous tests of the microscopic description, such as the calculation of elastic and inelastic cross sections, static nuclear properties, and electromagnetic transition rates.

A great many of these calculations involve the evaluation of reduced matrix elements of single-particle operators between initial and final nuclear states. For some of the more complicated nuclear models, this can be a formidable task; and, furthermore, the details vary from model to model.

If during evaluation of the matrix element, however, integration over the coordinates of the single-particle operator is left until last, the preceding integrations may be performed without any explicit reference to the single-particle operator. And, in fact, the result depends only on the initial and final states of the nucleus and on the nature of the transition involved. This leads directly to the concept of inelastic transition densities $\rho_{LSJ}^{if}(r)$, which essentially give, for the transition $i \rightarrow f$, the probability for absorption of angular momentum $J = L + S$ by the last nucleon as a function of its distance from the nuclear origin.

The idea of transition densities is not a new one. Such quantities were employed, for instance, by Haybron and McManus (ref. 1) in describing excitation of quadrupole and octupole levels of carbon-12 (^{12}C), oxygen-16 (^{16}O), and calcium-40 (^{40}Ca) using the particle-hole model, and by Gillet and Melkanoff (ref. 2) in describing inelastic electron scattering from the same nuclei. More recently, Glendenning (ref. 3) has developed a coupled-channel treatment of inelastic proton scattering using form factors which may be obtained from inelastic transition densities, and has emphasized that the coefficients needed for their calculation should be provided by the nuclear structure theorist. He gives examples for some currently popular nuclear models, and Braley and Ford (ref. 4) show how these coefficients may be constructed from projected Hartree-Fock wave functions. (These coefficients are essentially equivalent to the nuclear overlap coefficients $S_J(if|ab)$ of eq. (10).) Despite these occasional indications of interest, however, the convenience afforded by use of transition densities has been largely unnoticed.

In this report we attempt to provide a systematic description of the use of inelastic transition densities in calculating single-particle matrix elements. We find that these calculations are greatly simplified if the transition densities are expanded in terms of a biorthogonal set of functions which we call Gauss-Laguerre functions. Each density is then specified by a number of coefficients, and evaluation of any matrix element reduces to a simple sum over these coefficients. In order to be complete, we present all pertinent formulas, although some of these may be found elsewhere. Numerical examples for ^{20}Ne are also presented to serve as a test case for programs based on our results.

TRANSITION DENSITIES

Consider the matrix elements of an operator Ω between initial and final nuclear states,

$$\Omega_{if} = \langle J_f M_f | \Omega | J_i M_i \rangle \quad (1)$$

We define a generalized reduced matrix element of Ω by

$$\langle f || \Omega || i \rangle_{JM} \equiv \frac{\hat{J}^2}{\hat{J}_f^2} \sum_{M_i M_f} \langle J_i M_i, JM | J_f M_f \rangle \Omega_{if} \quad (2)$$

with M held fixed during the summation. (When Ω transforms like the M^{th} component of a spherical tensor of rank J , equation (2) reduces to the standard definition of ref. 5.) Inverting equation (2) yields

$$\Omega_{if} = \sum_{JM} \langle J_i M_i, JM | J_f M_f \rangle \langle f || \Omega || i \rangle_{JM} \quad (3)$$

Here $\langle J_i M_i, JM | J_f M_f \rangle$ is a Clebsch-Gordan coefficient and \hat{J} is shorthand for $\sqrt{2J+1}$.

Now suppose that Ω is a sum of single-particle operators,

$$\Omega = \sum_{n=1}^A \Omega(\vec{x}_n) \quad (4)$$

with $\vec{x}_n \equiv (r_n, \hat{x}_n)$ representing the radial and spin-angle coordinates of the n^{th} nucleon. We can isolate the dependence of the initial nuclear wave function on the coordinates of the n^{th} nucleon by making the expansion

$$|J_i M_i\rangle = A^{-1/2} \sum_{a m_a} \sum_{JM} \langle JM, j_a m_a | J_i M_i \rangle \psi_{a m_a}(\vec{x}_n) \Phi_{ia}^{JM}(\vec{x}_1 \dots \vec{x}_{n-1} \vec{x}_{n+1} \dots \vec{x}_A) \quad (5)$$

$$\psi_{a m_a}(\vec{x}) = \varphi_a(r) \vartheta_{l_a j_a}^{m_a}(\hat{x}) \quad (6)$$

$$\vartheta_{lj}^m(\hat{x}) = \sum_{m_l m_s} \left\langle l m_l, \frac{1}{2} m_s | j m \right\rangle Y_{l m_l}(\hat{r}) \chi_{1/2 m_s} \quad (7)$$

is a member of an appropriately chosen complete set of single-particle functions. The reduced matrix elements of Ω may now be expressed as

$$\langle f || \Omega || i \rangle_{JM} = \sum_{ab} S_J(if|ab) \langle b || \Omega || a \rangle_{JM} \quad (8)$$

where the generalized single-particle reduced matrix elements are given by

$$\langle b || \Omega || a \rangle_{JM} = \frac{J^2}{\hat{j}_b^2} \sum_{m_a m_b} \langle j_a m_a, JM | j_b m_b \rangle \langle b m_b | \Omega(\mathbf{x}) | a m_a \rangle \quad (9)$$

and the nuclear overlap coefficients $S_J(if|ab)$ by

$$S_J(if|ab) = \sum_{J'} U(j_a J' J J_f | J_i j_b) \langle \Phi_{fb}^{J'} || \Phi_{ia}^{J'} \rangle \quad (10)$$

with $U(abcd|ef) \equiv \hat{e}\hat{f}\hat{W}(abcd;ef)$. In the derivation, use is made of the relation (ref. 5)

$$\begin{aligned} \sum_{M_1} \langle j_1 m_1, j_2 m_2 | J_1 M_1 \rangle \langle J_1 M_1, j_3 m_3 | JM \rangle \\ = \sum_{J_2 M_2} \langle j_2 m_2, j_3 m_3 | J_2 M_2 \rangle \langle j_1 m_1, J_2 M_2 | JM \rangle U(j_1 j_2 J j_3 | J_1 J_2) \end{aligned} \quad (11)$$

and the orthogonality of the Clebsch-Gordan coefficients.

In most of the cases considered herein $\Omega(\vec{x})$ may be written

$$\Omega(\vec{x}) = \sum_{LSJM} \omega_{LSJM}(r) \mathcal{T}_{LSJ}(\hat{x}) \quad (12)$$

using the spin-angle tensors \mathcal{T}_{LSJ}^M defined by

$$\mathcal{T}_{LSJ}^M(\hat{x}) = \sum_{M_L M_S} \langle LM_L, SM_S | JM \rangle Y_{LM_L}(\hat{r}) \sigma_{SM_S} \quad (13)$$

(The operator σ_{SM_S} is a rank-S tensor in the spin-space of the particle; for spin-1/2 particles $\vec{\sigma}_0 = 1$ and $\vec{\sigma}_1 = 2\vec{S}$, where \vec{S} is the spin operator.) This permits the radial and spin-angle integrations to be performed separately:

$$\langle b || \Omega || a \rangle_{JM} = \sum_{LS} \langle j_b || \mathcal{T}_{LSJ} || j_a \rangle (\varphi_b | \omega_{LSJM} | \varphi_a) \quad (14)$$

(The spin-angle reduced matrix element in equation (14) is the standard one of ref. 5.)

Examining equations (8) and (14), we see that it is natural to define a set of $i \rightarrow f$ transition densities

$$\rho_{LSJ}^{if}(r) \equiv \sum_{ab} S_J(if|ab) \langle j_b || \mathcal{T}_{LSJ} || j_a \rangle \varphi_b^*(r) \varphi_a(r) \quad (15)$$

for then we have simply

$$\langle f || \Omega || i \rangle_{JM} = \sum_{LS} \langle f || \Omega || i \rangle_{LSJM} \quad (16)$$

$$\langle f || \Omega || i \rangle_{LSJM} = \int_0^\infty \rho_{LSJ}^{if}(r) \omega_{LSJM}(r) r^2 dr \quad (17)$$

EXPANSION IN GAUSS-LAGUERRE FUNCTIONS

To facilitate calculations involving the transition densities $\rho_{LSJ}^{if}(r)$, we expand them in terms of the very useful biorthogonal set of functions suggested by Sawaguri and Tobocman (ref. 6). These functions, which will be referred to as Gauss-Laguerre functions, have the following properties:

$$\mathcal{F}_{nL}(\alpha, \beta r) \equiv (\beta r)^L e^{-\alpha(\beta r)^2} \mathcal{L}_n^{L+1/2}(\beta^2 r^2) \quad (18)$$

$$\tilde{\mathcal{F}}_{nL}(\alpha, \beta r) = \left[\frac{2\beta^3 n!}{\Gamma\left(n + L + \frac{3}{2}\right)} \right] \mathcal{F}_{nL}(1 - \alpha, \beta r) \quad (19)$$

$$\int_0^\infty \mathcal{F}_{mL}(\alpha, \beta r) \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr = \delta_{mn} \quad (20)$$

$$\sum_{n=0} \mathcal{F}_{nL}(\alpha, \beta r) \tilde{\mathcal{F}}_{nL}(\alpha, \beta r') = \frac{\delta(r - r')}{r^2} \quad (21)$$

Here $\mathcal{L}_n^c(z)$ is a generalized Laguerre polynomial (ref. 7) of order \underline{c} and index \underline{n} . The Bessel transform of $\tilde{\mathcal{F}}_{nL}(\alpha, \beta r)$ is

$$\int_0^\infty j_L(kr) \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr = \beta^3 C_L(\alpha) \left(\frac{\alpha}{\alpha - 1} \right)^n \tilde{\mathcal{F}}_{nL}(1 - \alpha, \gamma k) \quad (22)$$

$$C_L(\alpha) = 2\sqrt{\pi} \alpha^{3/2+L/2} (1 - \alpha)^{-L/2} \quad (23)$$

$$\gamma = \left[2\beta \sqrt{\alpha(1 - \alpha)} \right]^{-1} \quad (24)$$

and in the limit $k \rightarrow 0$ this becomes

$$\int_0^\infty r^L \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr = \beta^{-L} (1 - \alpha)^{-L-3/2} \left(\frac{\alpha}{\alpha - 1} \right)^n \quad (25)$$

In terms of Gauss-Laguerre functions, the transition density may be written

$$\rho_{LSJ}^{\text{if}}(r) = \sum_{n=0}^\infty \rho_{LSJn}^{\text{if}} \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) \quad (26)$$

the coefficients being given by

$$\rho_{LSJn}^{\text{if}} = \int_0^\infty \rho_{LSJ}^{\text{if}}(r) \mathcal{F}_{nL}(\alpha, \beta r) r^2 dr \quad (27)$$

This leads directly to our basic result,

$$\langle f || \Omega || i \rangle_{LSJM} = \sum_{n=0}^\infty \rho_{LSJn}^{\text{if}} \int_0^\infty \omega_{LSJM}(r) \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr \quad (28)$$

The significance of equation (28) is that the radial integral involving ω_{LSJM} and \mathcal{F}_{nL} may be done analytically, in closed form, and thus for any Ω the evaluation of $\langle f || \Omega || i \rangle_{\text{LSJM}}$ is reduced to a relatively simple sum over the coefficients $\rho_{\text{LSJn}}^{\text{if}}$.

ILLUSTRATIONS

Suppose, for instance, that we wish to calculate some static nuclear properties. First, it is necessary to check the wave function normalization, that is, to evaluate

$$\langle J_i M_i | J_i M_i \rangle = \langle i || 1 || i \rangle_{00} \quad (29)$$

Here the operator Ω is

$$\Omega = 1 = \sum_{n=1}^A \frac{1}{A} = \sum_{n=1}^A \sum_{\text{LSJM}} \mathcal{T}_{\text{LSJ}}(\hat{x}_n) \left[\frac{\sqrt{4\pi}}{A} \delta_{L0} \delta_{S0} \right] \quad (30)$$

Hence,

$$\omega_{\text{LSJM}}(r) = \frac{\sqrt{4\pi}}{A} \delta_{L0} \delta_{S0} \quad (31)$$

Using equation (25) with $L = 0$ in equation (28), we find that

$$\langle i || 1 || i \rangle_{00} = \frac{\sqrt{4\pi}}{A} (1 - \alpha)^{-3/2} \sum_{n=0}^{\infty} \left(\frac{\alpha}{\alpha - 1} \right)^n \rho_{000n}^{\text{if}} \quad (32)$$

It will turn out that $\rho_{\text{LSJn}}^{\text{if}}$ is nearly always accompanied by the factor $[\alpha/(\alpha - 1)]^n$, and so we define

$$\tilde{\rho}_{\text{LSJn}}^{\text{if}} \equiv \left(\frac{\alpha}{\alpha - 1} \right)^n \rho_{\text{LSJn}}^{\text{if}} \quad (33)$$

Hence,

$$\langle J_i M_i | J_i M_i \rangle = \frac{\sqrt{4\pi}}{A} (1 - \alpha)^{-3/2} \sum_{n=0}^{\infty} \tilde{\rho}_{000n}^{ii} \quad (34)$$

Since

$$r^2 \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) = \frac{1}{\beta^2} \frac{\partial}{\partial \alpha} \tilde{\mathcal{F}}_{nL}(\alpha, \beta r)$$

differentiation of equation (25) with respect to α may be used to evaluate the integral involving

$$\omega_{LSJM}(r) = \frac{\sqrt{4\pi}}{A} r^2 \delta_{L0} \delta_{S0} \quad (35)$$

From this we deduce the following expression for the mean square matter radius:

$$\left\langle J_i M_i \left| \frac{1}{A} \sum_{n=1}^A r_n^2 \right| J_i M_i \right\rangle = \frac{\sqrt{4\pi}}{A\beta^2} (1 - \alpha)^{-5/2} \sum_{n=0}^{\infty} \left(\frac{n}{\alpha} + \frac{3}{2} \right) \tilde{\rho}_{000n}^{ii} \quad (36)$$

To obtain the electric quadrupole moment Q of the nucleus, we must evaluate $\langle i || \Omega || i \rangle_{20}$, where

$$\Omega = e \left(\frac{16\pi}{5} \right)^{1/2} \sum_{n=1}^A r_n^2 Y_{20}(\hat{r}_n) \left(\frac{1 + \tau_n}{2} \right) \quad (37)$$

and τ_n is the z-component of the isospin operator for the n^{th} nucleon. Comparison of equations (37) and (12) shows that for this case

$$\omega_{LSJM}(r) = e \left(\frac{16\pi}{5} \right)^{1/2} r^2 \left(\frac{1 + \tau}{2} \right) \delta_{L2} \delta_{S0} \quad (38)$$

Since the operator $(1 + \tau)/2$ picks out the proton part $\rho_{\text{LSJ}}^{\text{p}}(\mathbf{r})$ of the transition density

$$\rho_{\text{LSJ}}(\mathbf{r}) = \rho_{\text{LSJ}}^{\text{p}}(\mathbf{r}) + \rho_{\text{LSJ}}^{\text{n}}(\mathbf{r}) \quad (39)$$

(the superscript if will be dropped for clarity when necessary), use of equation (25) with $L = 2$ in equation (28) yields

$$Q = e^{\left(\frac{16\pi}{5}\right)^{1/2}} \beta^{-2} (1 - \alpha)^{-7/2} \sum_{n=0}^{\infty} \tilde{\rho}_{202n}^{\text{p}} \quad (40)$$

To conclude this section, let us evaluate some simple dynamic nuclear properties. Here we are usually concerned with the absolute square of the matrix element Ω_{if} , averaged over initial states and summed over final states:

$$\frac{1}{\hat{J}_i^2} \sum_{M_i M_f} \left| \Omega_{\text{if}} \right|^2 = \frac{\hat{J}_f^2}{\hat{J}_i^2} \sum_{JM} \frac{1}{\hat{J}^2} \left| \langle f || \Omega || i \rangle_{JM} \right|^2 \quad (41)$$

Consider, for example, the reduced electromagnetic transition probability $B(E\lambda)$ for the $i \rightarrow f$ transition. Here the operator Ω is given by

$$\Omega = e \sum_{n=1}^A r_n^{\lambda} Y_{\lambda\mu}(\hat{\mathbf{r}}_n) \left(\frac{1 + \tau_n}{2} \right) \quad (42)$$

and the sum over final states includes a sum (not shown above) over the photon orientation μ . In this case, the reduced matrix element is independent of μ , so that the sum over μ gives a factor of $\lambda^2 (= J^2)$; use of equation (25) then yields

$$B(E\lambda) = \frac{\hat{J}_f^2}{\hat{J}_i^2} \left| \beta^{-\lambda} (1 - \alpha)^{-\lambda-3/2} \sum_{n=0}^{\infty} \tilde{\rho}_{\lambda 0 \lambda n}^{\text{p}} \right|^2 \quad (43)$$

As an example of a case where ω_{LSJM} (and hence the generalized reduced matrix element) depends explicitly on M , let us evaluate the Born approximation electron scattering form factor $|F(q)|^2$, which is defined as above with

$$\Omega = \frac{1}{Z} \sum_{n=1}^A e^{i\vec{q} \cdot \vec{r}_n} \left(\frac{1 + \tau_n}{2} \right) \quad (44)$$

Here we have

$$\omega_{\text{LSJM}}(r) = \frac{4\pi}{Z} i^{L_j} j_L(qr) Y_{LM}^*(\hat{q}) \left(\frac{1 + \tau}{2} \right) \delta_{S0} \delta_{LJ} \quad (45)$$

and so (using eq. (22))

$$|F(\vec{q})|^2 = \frac{j_f^2}{j_i^2} \sum_{LM} \frac{1}{\hat{L}^2} \left| \sum_{n=0}^{\infty} \tilde{\rho}_{L0Ln}^p \frac{4\pi}{Z} i^{L_Y} Y_{LM}^*(\hat{q}) \beta^3 C_L(\alpha) \tilde{\mathcal{F}}_{nL}(1 - \alpha, \gamma q) \right|^2 \quad (46)$$

The sum over M is readily carried out by using the addition theorem for spherical harmonics, yielding

$$|F(q)|^2 = \frac{\hat{j}_f^2}{\hat{j}_i^2} \sum_L 4\pi \left| \frac{\beta^3}{Z} C_L(\alpha) \sum_{n=0}^{\infty} \tilde{\rho}_{L0Ln}^p \tilde{\mathcal{F}}_{nL}(1 - \alpha, \gamma q) \right|^2 \quad (47)$$

Equation (47) does not contain modifications which arise when the finite size of the proton charge distribution is considered. These are treated in appendix A.

NUCLEON SCATTERING FORM FACTOR

A more complicated application occurs in the analysis of inelastic nucleon scattering, where we need reduced matrix elements of (for example) a central nucleon-nucleon interaction

$$V = \sum_{n=1}^A V(\vec{x}_n, \vec{x}_0) \quad (48)$$

where \vec{x}_0 denotes the projectile coordinates and

$$V(\vec{x}_n, \vec{x}_0) = \sum_{S=0}^1 V_S(|\vec{r}_0 - \vec{r}_n|) \vec{\sigma}_S(0) \cdot \vec{\sigma}_S(n) \quad (49)$$

Following Tobocman, we introduce the Fourier transform of V_S :

$$V_S(|\vec{r}_0 - \vec{r}_n|) = (2\pi)^{-3} \int V_S(k) e^{i\vec{k} \cdot \vec{r}_0} e^{-i\vec{k} \cdot \vec{r}_n} d\vec{k} \quad (50)$$

If each plane wave is expanded in spherical harmonics, the angular integration over \hat{k} is trivial and leads to

$$V(\vec{x}_n, \vec{x}_0) = \left(\frac{2}{\pi}\right) \sum_{LSJM} (-1)^{L+S+J+M} \mathcal{Y}_{LSJ}^M(\hat{x}_n) \mathcal{Y}_{LSJ}^{-M}(\hat{x}_0) \int_0^\infty V_S(k) j_L(kr_0) j_L(kr_n) k^2 dk \quad (51)$$

By comparing this with equation (12) we can identify ω_{SLJM} ; then from equation (28) we have

$$\langle f || V || i \rangle_{LSJM} = (-1)^{L+S+J+M} \mathcal{Y}_{LSJ}^{-M}(\hat{x}_0) f_{LSJ}(r_0) \quad (52)$$

where the nucleon scattering form factor $f_{LSJ}(r_0)$ is given by

$$f_{LSJ}(r_0) = \left(\frac{2}{\pi}\right) \sum_{n=0}^\infty \rho_{LSJn}^{\text{if}} \int_0^\infty r^2 dr \mathcal{F}_{nL}(\alpha, \beta r) \int_0^\infty V_S(k) j_L(kr_0) j_L(kr) k^2 dk \quad (53)$$

To evaluate $f_{LSJ}(r_0)$, we first carry out the integration over \underline{r} by means of equation (22):

$$f_{LSJ}(r_0) = \left(\frac{2}{\pi}\right) \beta^3 C_L(\alpha) \sum_{n=0}^\infty \tilde{\rho}_{LSJn}^{\text{if}} \int_0^\infty V_S(k) j_L(kr_0) \tilde{\mathcal{F}}_{nL}(1 - \alpha, \gamma k) k^2 dk \quad (54)$$

Next suppose that $V_S(r)$ can be expanded in Gauss-Laguerre functions,

$$V_S(r) = \sum_{m=0}^{\infty} V_{Sm} \tilde{\mathcal{F}}_{m0}(\alpha', \beta' r) \quad (55)$$

$$V_{Sm} = \int_0^{\infty} V_S(r) \mathcal{F}_{m0}(\alpha', \beta' r) r^2 dr \quad (56)$$

The choice $L = 0$ is appropriate because of the central nature of V_S . Again using equation (22), we find

$$v_S(k) = 4\pi\beta'^3 C_0(\alpha') \sum_{m=0}^{\infty} \tilde{V}_{Sm} \tilde{\mathcal{F}}_{m0}(1 - \alpha', \gamma' k) \quad (57)$$

This leaves us with

$$\begin{aligned} f_{LSJ}(r_0) &= 8(\beta\beta')^3 C_L(\alpha) C_0(\alpha') \sum_{n=0}^{\infty} \tilde{\rho}_{LSJn}^{if} \sum_{m=0}^{\infty} \tilde{V}_{Sm} \\ &\times \int_0^{\infty} j_L(kr_0) \tilde{\mathcal{F}}_{nL}(1 - \alpha, \gamma k) \tilde{\mathcal{F}}_{m0}(1 - \alpha', \gamma' k) k^2 dk \end{aligned} \quad (58)$$

The last step in the analysis is to observe that the product of the two Gauss-Laguerre functions may be written in the form

$$\mathcal{F}_{nL}(1 - \alpha, \gamma k) \mathcal{F}_{m0}(1 - \alpha', \gamma' k) = k^L e^{-k^2/4\zeta^2} \sum_{N=0}^{m+n} Q_{mnN}^L k^{2N} \quad (59)$$

where

$$\frac{1}{\zeta^2} = 4\alpha\gamma^2 + 4\alpha'\gamma'^2 \quad (60)$$

The coefficient Q_{mnN}^L is obtained by multiplying together the two series expansions for the Gauss-Laguerre functions, the result being

$$Q_{mnN}^L = \left[\frac{8(\gamma\gamma')^3 \gamma^{2N+L}}{\sqrt{\pi} \Gamma\left(N + L + \frac{3}{2}\right)} \right] (-1)^N \sum_{K=0}^N \frac{\left(-N - L - \frac{1}{2}\right)_K}{\left(\frac{3}{2}\right)_K} (-1)^K \binom{m}{K} \binom{n}{N-K} \left(\frac{\gamma'}{\gamma}\right)^{2K} \quad (61)$$

The integration over k may now be carried out with the help of

$$\int_0^\infty k^{2N+L} e^{-k^2/4\zeta^2} j_L(kr_0) k^2 dk = \frac{1}{4} \sqrt{\pi} N! (2\zeta)^{2N+L+3} \mathcal{F}_{NL}(1, \zeta r_0) \quad (62)$$

This yields an expression for $f_{LSJ}(r_0)$ which, after some rearranging, may be written

$$f_{LSJ}(r_0) = \sum_{N=0}^{\infty} f_{LSJN} \tilde{\mathcal{F}}_{NL}(0, \zeta r_0) \quad (63)$$

where the form factor coefficients f_{LSJN} are given by

$$f_{LSJN} = C_L(\alpha) C_0(\alpha') \left[\alpha \alpha' (1 - \alpha)(1 - \alpha') \right]^{-3/2} (-1)^N (2\gamma\zeta)^{2N+L} \sum_{K=0}^N \frac{\left(-N - L - \frac{1}{2}\right)_K}{\left(\frac{3}{2}\right)_K} \times (-1)^K \left(\frac{\gamma'}{\gamma}\right)^{2K} \left[\sum_{n=0}^{\infty} \tilde{\rho}_{LSJn}^{\text{if}} \binom{n}{N-K} \right] \left[\sum_{m=0}^{\infty} \tilde{v}_{Sm} \binom{m}{K} \right] \quad (64)$$

Although the series above look somewhat formidable, they are easily handled by the computer and, in practice, converge quite rapidly for short-range forces. (The exceptional case of the long-range Coulomb force is treated in appendix B.) Only the $m = 0$ term is necessary if $V_S(r)$ has Gaussian shape, for instance, and only a few values of ρ_{LSJn}^{if} are nonzero if harmonic oscillator single-particle functions are used.

Even when the more realistic Wood-Saxon single-particle functions are used, it is demonstrated in appendix C that an accurate description of $\rho_{\text{LSJ}}^{\text{if}}(r)$ is provided with about 20 terms.

PRACTICAL CONSIDERATIONS

From the foregoing analysis, there emerges a straightforward recipe for calculating matrix elements of single-particle operators from a knowledge of the nuclear wave functions:

- (1) The overlap coefficients $S_J(\text{if}|ab)$ are obtained, and then, by means of equation (15), the transition densities $\rho_{\text{LSJ}}^{\text{if}}(r)$.
- (2) The densities are expanded in a series of Gauss-Laguerre functions, whose coefficients are obtained by means of equation (27).
- (3) The coefficients $\rho_{\text{LSJn}}^{\text{if}}$ may then be used in relatively simple formulas to obtain the desired matrix elements.

In this section we shall discuss some of the practical aspects of this recipe.

To begin with, the symmetry properties of the overlap coefficients can be simplified by defining a related coefficient

$$\begin{aligned}\tilde{S}_J(\text{if}|ab) &\equiv \sum_{J'} W(j_a J' J J_f; J_i j_b) \langle \Phi_{fb}^{J'} \| \Phi_{ia}^{J'} \rangle \\ &= \frac{S_J(\text{if}|ab)}{\hat{j}_i \hat{j}_b}\end{aligned}\tag{65}$$

for then

$$\tilde{S}_J(\text{fi}|ba) = (-1)^{j_a - j_b + J_f - J_i} \tilde{S}_J(\text{if}|ab)\tag{66}$$

(The \tilde{S}_J are the nuclear structure coefficients discussed by Glendenning.)

The reduced matrix element of the tensor $\mathcal{T}_{\text{LSJ}}^M$, which is needed for constructing the transition densities by means of equation (15), is conveniently expressed in terms of the quantity

$$g_{\text{LSJ}}^{ab} \equiv \frac{\sqrt{4\pi}}{\hat{j}_a} (-1)^{j_a + (1/2)} \langle j_b \| \mathcal{T}_{\text{LSJ}} \| j_a \rangle\tag{67}$$

which has the symmetry property

$$g_{LSJ}^{ba} = (-1)^{L+S+J} g_{LSJ}^{ab} \quad (68)$$

When triangle inequalities are satisfied by the triads (l_a, l_b, L) , (j_a, j_b, J) , and (L, S, J) , and the sum $(l_a + l_b + L)$ is even, g_{LSJ}^{ab} is given by

$$g_{L0L}^{ab} = \left\langle j_a - \frac{1}{2}, j_b \frac{1}{2} \middle| J0 \right\rangle \quad (69)$$

$$g_{L1L}^{ab} = (-1)^{l_a+1/2+j_a} \left\langle j_a \frac{1}{2}, j_b \frac{1}{2} \middle| J1 \right\rangle \quad (70)$$

$$g_{L1L\pm 1}^{ab} = \frac{g_{L0L}^{ab} (B \mp A)}{\hat{J} \sqrt{A}} \quad (71)$$

where $A = (L + J + 1)/2$, $B = \lambda_a + \lambda_b$, and $\lambda = (l - j)(2l + 1) - (1/2)$; otherwise g_{LSJ}^{ab} vanishes.

Some care must be taken in generating the Gauss-Laguerre functions to avoid excessive roundoff error. A simple, but highly accurate, scheme based on the recursion relation satisfied by the functions is as follows: Let $\varphi_0 = 1$ and $\Delta_0 = 0$, and calculate

$$S_n = \left(L - \frac{1}{2} \right) \Delta_n - (\beta r)^2 \varphi_n \quad (72)$$

$$\varphi_{n+1} = \varphi_n + \Delta_n + (n + 1)^{-1} S_n \quad (73)$$

$$\Delta_{n+1} = \varphi_{n+1} - \varphi_n \quad (74)$$

Then

$$\mathcal{J}_{nL}(\alpha, \beta r) = (\beta r)^L e^{-\alpha(\beta r)^2} \varphi_n \quad (75)$$

To evaluate the sum of a series of Gauss-Laguerre functions, let $\varphi_{N+1} = \Delta_{N+1} = 0$ and calculate

$$S_n = A_n + \left(L + \frac{3}{2}\right)\Delta_{n+1} - (\beta r)^2 \varphi_{n+1} \quad (76)$$

$$\varphi_n = \varphi_{n+1} + \Delta_{n+1} + n^{-1}S_n \quad (77)$$

$$\Delta_n = \varphi_n - \varphi_{n+1} \quad (78)$$

Then

$$\sum_{n=0}^N A_n \mathcal{F}_{nL}(\alpha, \beta r) = (\beta r)^L e^{-\alpha(\beta r)^2} S_0 \quad (79)$$

Similar formulas may be developed for the functions $\tilde{\mathcal{F}}_{nL}(\alpha, \beta r)$. For large values of βr , double-precision arithmetic may be required.

It is desirable to calculate the coefficients ρ_{LSJn}^{if} by direct numerical integration of $\rho_{LSJ}^{\text{if}}(r)$ (although this could be avoided if harmonic oscillator single-particle functions were used), for the method is then independent of the choice of the set $\varphi_a(r)$. The number of terms needed can be determined by comparing the original density $\rho_{LSJ}^{\text{if}}(r)$ with the truncated Gauss-Laguerre series representation. When harmonic oscillator single-particle functions are used, of course, $\rho_{LSJ}^{\text{if}}(r)$ will be a polynomial in r^2 times a factor of the form $\exp(-\nu r^2)$; hence, in this case, truncation error can be avoided completely by putting $(1 - \alpha)\beta^2 = \nu$.

If nucleon scattering form factors $f_{LSJ}(r_0)$ are desired, it is necessary to calculate the coefficients V_{Sm} . When the potential has terms of Gaussian shape, the following integral may be used:

$$\int_0^\infty r^L e^{-r^2/R^2} \mathcal{F}_{mL}(\alpha', \beta' r) r^2 dr = \frac{\Gamma\left(m + L + \frac{3}{2}\right)}{2m! y^3} \left(\frac{\beta'}{y^2}\right)^L \left(1 - \frac{\beta'^2}{y^2}\right)^m \quad (80)$$

with $L = 0$, where $y^2 = \alpha'\beta'^2 + R^{-2}$. Only the $m = 0$ term is nonzero if the parameters are adjusted so that $y = \beta'$, that is, $(1 - \alpha')\beta'^2 = R^{-2}$. If it is desired to employ several potentials with different ranges using only one parameter set, it is best to choose $y = \beta'$ for the largest range.

The Yukawa force

$$V_S(r) = V_0 \frac{e^{-r/R}}{r} \quad (81)$$

presents some problems, for good convergence of the series for $V_S(r)$ cannot be expected. Fortunately, all that is really required is that α' and β' be selected so that the series (eq. (57)) for $v_S(k)$ is accurate enough for use in equation (54). The first two coefficients in this series are given by

$$V_{S0} = \left(\frac{V_0}{\alpha' \beta'^2} \right) \left[\frac{1}{2} - x e^{-x^2} \text{Erfc}(x) \right] \quad (82)$$

$$V_{S1} = \left(\frac{3}{2} + \frac{\partial}{\partial \alpha'} \right) V_{S0} \quad (83)$$

where $x = (2\beta'R \sqrt{\alpha'})^{-1}$, and the rest satisfy

$$V_{Sm+1} = V_{Sm} + \left(\frac{\alpha' - 1}{\alpha'} \right) (V_{Sm} - V_{Sm-1}) + \frac{1}{n+1} \left[\left(\frac{1}{\alpha' \beta' R} - \frac{1}{2} \right) V_{Sm} + \frac{\alpha' - 1}{\alpha'} V_{Sm-1} \right] \quad (84)$$

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, April 13, 1970,
129-02.

APPENDIX A

EFFECTS OF DISTRIBUTED NUCLEON CHARGE

When the operator $\Omega(\vec{x})$ arises from the interaction between an electron and the nucleon at \vec{x} , it should be replaced by

$$\Omega_C(\vec{x}) = \int \rho_C(\vec{r} - \vec{r}') \Omega(\vec{x}') d\vec{r}' \quad (A1)$$

where ρ_C represents the charge distribution of the nucleon. In this section, we shall indicate how this modification may be accomplished by simple changes in α, β , and ρ_{LSJn}^{if} .

Suppose, for example, that only the proton is to be considered charged, and its distribution is to be Gaussian with an rms radius of R_p :

$$\rho_C(\vec{r} - \vec{r}') = (2\pi)^{-3} \int e^{i\vec{k} \cdot \vec{r}} e^{-i\vec{k} \cdot \vec{r}'} e^{-(1/6)k^2 R_p^2} d\vec{k} \quad (A2)$$

Then if $\Omega(\vec{x})$ possesses the expansion (eq. (12)), it can easily be shown by expanding the plane waves in equation (A2) that

$$\Omega_C(\vec{x}) = \sum_{LSJM} \omega_{LSJM}^C(r) \mathcal{F}_{LSJ}^M(\hat{x}) \quad (A3)$$

where

$$\omega_{LSJM}^C(r) = \left(\frac{2}{\pi}\right) \int_0^\infty k^2 dk j_L(kr) e^{-(1/6)k^2 R_p^2} \int_0^\infty j_L(kr') \omega_{LSJM}(r') r'^2 dr' \quad (A4)$$

(It is understood that $\omega_{LSJM}(r')$ contains the factor $(1 + \tau)/2$.)

Now in evaluating a reduced matrix element of Ω by means of equation (28), we encounter the integral

$$I = \int_0^\infty \omega_{LSJM}^C(r) \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr \quad (A5)$$

With the substitution of equation (A4) for $\omega_{\text{LSJM}}^{\text{C}}(\mathbf{r})$, the integration over $\underline{\mathbf{r}}$ may be carried out by means of equation (22), leaving

$$I = \left(\frac{2}{\pi}\right) \beta^3 C_0(\alpha) \left(\frac{\alpha}{\alpha - 1}\right)^n \int_0^\infty k^2 dk e^{-(1/6)k^2 R_p^2} \tilde{\mathcal{F}}_{\text{nL}}(1 - \alpha, \gamma k) \int_0^\infty j_L(kr') \omega_{\text{LSJM}}(\mathbf{r}') r'^2 dr' \quad (\text{A6})$$

Next we observe that

$$e^{-(1/6)k^2 R_p^2} \tilde{\mathcal{F}}_{\text{nL}}(1 - \alpha, \gamma k) = \tilde{\mathcal{F}}_{\text{nL}}(1 - \alpha_{\text{C}}, \gamma k) \quad (\text{A7})$$

where

$$\alpha_{\text{C}} = \alpha + \frac{R_p^2}{6\gamma^2} = \alpha \left[1 + \frac{2}{3} (1 - \alpha) (\beta R_p)^2 \right] \quad (\text{A8})$$

with γ unchanged. A second application of equation (22) (this time to the $\underline{\mathbf{k}}$ -integration) then yields

$$I = D_{\text{nL}} \int_0^\infty \omega_{\text{LSJM}}(\mathbf{r}') \tilde{\mathcal{F}}_{\text{nL}}(\alpha_{\text{C}}, \beta_{\text{C}} r') r'^2 dr' \quad (\text{A9})$$

where

$$\beta_{\text{C}} = \left[2\gamma \sqrt{\alpha_{\text{C}}(1 - \alpha_{\text{C}})} \right]^{-1} = \beta \sqrt{\frac{\alpha(1 - \alpha)}{\alpha_{\text{C}}(1 - \alpha_{\text{C}})}} \quad (\text{A10})$$

$$D_{\text{nL}} = \left(\frac{\alpha}{\alpha_{\text{C}}}\right)^{n+(L/2)} \left(\frac{1 - \alpha_{\text{C}}}{1 - \alpha}\right)^{n+(L/2)+(3/2)} \quad (\text{A11})$$

Comparison of equations (A5) and (A9) shows that the effect of using $\omega_{\text{LSJM}}^{\text{C}}(\mathbf{r})$ instead of $\omega_{\text{LSJM}}(\mathbf{r})$ in evaluating I is equivalent to carrying out the latter evaluation with parameter values α_{C} and β_{C} and then inserting the factor D_{nL} . Consequently,

all subsequent formulas (such as eq. (46) for $|F(\vec{q})|^2$, for example) remain valid if the replacements

$$\left. \begin{aligned} \alpha &\rightarrow \alpha_C \\ \beta &\rightarrow \beta_C \\ \rho_{\text{LSJn}}^{\text{if}} &\rightarrow D_{\text{nL}} \rho_{\text{LSJn}}^{\text{if}} \end{aligned} \right\} \quad (\text{A12})$$

are made throughout.

It is instructive to apply this method to obtain the mean square nuclear charge radius. Writing

$$\Omega = \frac{1}{Z} \sum_{n=1}^A r_n^2 \left(\frac{1 + \tau_n}{2} \right) \quad (\text{A13})$$

we obtain (cf. eq. (36))

$$\langle J_i M_i | \Omega | J_i M_i \rangle = \frac{\sqrt{4\pi}}{Z} \beta^{-2} (1 - \alpha)^{-5/2} \sum_{n=0}^{\infty} \left(\frac{n}{\alpha} + \frac{3}{2} \right) \tilde{\rho}_{000n}^p \quad (\text{A14})$$

After the substitutions noted in equation (A12) are made throughout, the resulting expression simplifies to

$$\langle J_i M_i | \Omega_C | J_i M_i \rangle = \langle J_i M_i | \Omega | J_i M_i \rangle + \frac{\sqrt{4\pi}}{Z} \beta^{-2} (1 - \alpha)^{-5/2} \frac{3}{2} \left(\frac{\alpha_C}{\alpha} - 1 \right) \sum_{n=0}^{\infty} \tilde{\rho}_{000n}^p \quad (\text{A15})$$

To evaluate the sum over $\tilde{\rho}_{000n}^p$, consider the following (cf. eq. (34)):

$$1 = \left\langle J_i M_i \left| \frac{1}{Z} \sum_{n=1}^A \left(\frac{1 + \tau_n}{2} \right) \right| J_i M_i \right\rangle = \frac{\sqrt{4\pi}}{Z} (1 - \alpha)^{-3/2} \sum_{n=0}^{\infty} \tilde{\rho}_{000n}^p \quad (\text{A16})$$

Using this and equation (A8) in equation (A15) we find that

$$\langle J_i M_i | \Omega_C | J_i M_i \rangle = \langle J_i M_i | \Omega | J_i M_i \rangle + R_p^2 \quad (\text{A17})$$

as expected.

APPENDIX B

COULOMB FORM FACTORS

For the long-range Coulomb force

$$V(\vec{x}_0, \vec{x}_n) = \frac{e^2}{|\vec{r}_0 - \vec{r}_n|} \left(\frac{1 + \tau_n}{2} \right) \quad (B1)$$

the series derived earlier for nucleon scattering form factors converge only conditionally, and a different method should be used. We begin with the familiar multipole expansion of $|\vec{r}_0 - \vec{r}_n|^{-1}$, which leads to

$$\langle f || V || i \rangle_{\mathbf{LSJM}} = Y_{LM}^*(\hat{r}_0) f_L(r_0) \delta_{S0} \delta_{LJ} \quad (B2)$$

$$f_L(r_0) = \frac{4\pi}{2L+1} e^2 \sum_{n=0}^{\infty} \rho_{L0Ln}^p \int_0^{\infty} r_{< r >}^{L-L-1} \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr \quad (B3)$$

where $r_{< r >}$ is the smaller (larger) of (r_0, r) .

Consider first the integral

$$I_n(r_0) = r_0^{-L-1} \int_0^{r_0} r^L \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr \quad (B4)$$

$$= \frac{1}{r_0} (\beta r_0)^{-L} \varphi_n(\beta^2 r_0^2) \quad (B5)$$

where

$$\varphi_n(x) = \int_0^x e^{-(1-\alpha)y} \psi_n^L(y) dy \quad (B6)$$

and

$$\psi_n^L(y) = y^{L+(1/2)} {}_1F_1 \left(\begin{matrix} -n; L + \frac{3}{2}; y \end{matrix} \right) \frac{1}{\Gamma\left(L + \frac{3}{2}\right)} \quad (B7)$$

Now it can be shown (ref. 7) that

$$\int \psi_n^L(y) dy = \psi_n^{L+1}(y) = \psi_n^L(y) - \psi_{n+1}^L(y) \quad (B8)$$

Thus, integrating equation (B6) by parts gives

$$\varphi_n(x) = e^{-(1-\alpha)x} \psi_n^{L+1}(x) + (1 - \alpha) [\varphi_n(x) - \varphi_{n+1}(x)] \quad (B9)$$

This two-term recursion relation for $\varphi_n(x)$ is readily solved, yielding

$$\varphi_n(x) = \left(\frac{\alpha}{\alpha - 1} \right)^n \left[\varphi_0(x) - \frac{1}{\alpha} \sum_{m=0}^{n-1} \left(\frac{\alpha - 1}{\alpha} \right)^m e^{-(1-\alpha)x} \psi_m^{L+1}(x) \right] \quad (B10)$$

Consequently, the integral $I_n(r_0)$ may be written

$$I_n(r_0) = \left(\frac{\alpha}{\alpha - 1} \right)^n \left[I_0(r_0) - \frac{r_0}{2\alpha\beta} \sum_{m=0}^{n-1} \left(\frac{\alpha - 1}{\alpha} \right)^m \tilde{\mathcal{F}}_{mL+1}(\alpha, \beta r_0) \right] \quad (B11)$$

The integral $I_0(r_0)$ cannot be put into elementary form, but a change of variable so that the limits of integration are 0 and 1 leads to

$$I_0(r_0) = \frac{1}{r_0} (\beta r_0)^{L+3} e^{-x} {}_1F_1 \left(\begin{matrix} 1; L + \frac{5}{2}; x \end{matrix} \right) \frac{1}{\Gamma\left(L + \frac{5}{2}\right)} \quad (B12)$$

where $x = (1 - \alpha)(\beta r_0)^2$. For small x , the confluent hypergeometric function may be developed in a power series. For larger x , the following equation may be used:

$$I_0(r_0) = \frac{1}{r_0} (\beta r_0)^{L+3} \left[\frac{\text{Erf}(\sqrt{x})}{x^{L+(3/2)} \Gamma\left(\frac{3}{2}\right)} - \frac{e^{-x}}{x} \sum_{k=0}^L \frac{x^{-L+k}}{\Gamma\left(k + \frac{3}{2}\right)} \right] \quad (\text{B13})$$

Next we turn to the integral

$$K_n(r_0) = r_0^L \int_{r_0}^{\infty} r^{-L-1} \tilde{\mathcal{F}}_{nL}(\alpha, \beta r) r^2 dr \quad (\text{B14})$$

$$= \frac{1}{r_0} (\beta r_0)^{L+1} \frac{n!}{\Gamma\left(n + L + \frac{3}{2}\right)} \varphi_n(\beta^2 r_0^2) \quad (\text{B15})$$

where now

$$\varphi_n(x) = \int_x^{\infty} e^{\alpha y} \psi_n^L(y) dy \quad (\text{B16})$$

with

$$\psi_n^L(y) = e^{-y} \mathcal{L}_n^{L+(1/2)}(y) \quad (\text{B17})$$

In this case, $\psi_n^L(y)$ satisfies

$$\int \psi_n^L(y) dy = -\psi_n^{L-1}(y) = \psi_{n-1}^L(y) - \psi_n^L(y) \quad (\text{B18})$$

and so proceeding much as before we find that

$$\varphi_n(x) = \left(\frac{\alpha}{\alpha - 1} \right)^n \left[\varphi_0(x) + \frac{1}{1 - \alpha} \sum_{m=1}^n \left(\frac{\alpha - 1}{\alpha} \right)^m e^{\alpha x} \psi_m^{L-1}(x) \right] \quad (\text{B19})$$

In this case, $\varphi_0(x)$ can be easily evaluated, with the result

$$K_n(r_0) = \frac{n!}{\Gamma\left(n + L + \frac{3}{2}\right)} \left(\frac{\alpha}{\alpha - 1}\right)^n \frac{\beta^2 r_0}{1 - \alpha} \sum_{m=0}^n \left(\frac{\alpha - 1}{\alpha}\right)^m \mathcal{J}_{mL-1}(1 - \alpha, \beta r_0) \quad (B20)$$

APPENDIX C

NUMERICAL EXAMPLES

To illustrate parameter values for a typical case, we present some numerical results for ^{20}Ne as examples of the various formulas given previously. These results are representative only, and are not intended as a serious effort to reproduce the experimental data.

The nuclear wave functions were projected from axially symmetric intrinsic Hartree-Fock states with 20 orbits, employing for the most part harmonic oscillator single-particle functions spanning the 1s, 1p, 2s-1d, and 2p-1f shells. From these wave functions the nuclear overlap coefficients $S_J(\text{if}|\text{ab})$ were determined by the methods of reference 4. These overlap coefficients, which are listed in table I, form the point of departure for the results given in the following paragraphs.

Using a modified Simpson's rule algorithm with end-point corrections, with 100 intervals of 0.1 fm width, the density coefficients $\rho_{\text{LSJn}}^{\text{if}}$ were computed numerically for the elastic $0^+ \rightarrow 0^+$ transition and the inelastic $0^+ \rightarrow 2^+$ transition. The values $\alpha = 0.5593$ and $\beta = 0.8 \text{ fm}^{-1}$ were chosen to match roughly the harmonic oscillator parameter $\nu = 0.282 \text{ fm}^{-2}$. The density coefficients are listed in table II; nonzero values for $n \geq 2$ (LSJ = 000) and $n \geq 3$ (LSJ = 202, 212) are indicative of roundoff and truncation errors, but they are gratifyingly small.

In table III we give the calculated and experimental nuclear matter radius and transition rate $B(E2)$, and in table IV the Born approximation electron scattering form factors for selected values of q^2 . For the nucleon scattering form factors, the Glendenning-Veneroni force (ref. 8) was used:

$$V(\vec{x}) = -52.0 \text{ e}^{-(r/1.85)^2} (P_{\text{TE}} + 0.6 P_{\text{SE}}) \quad (\text{C1})$$

Here we used $\beta' = 1$ and adjusted α' so that only V_{S0} was nonzero. The form factor coefficients f_{LSJN} are listed in table V.

As a last example, we consider a Hartree-Fock wave function for ^{20}Ne using Wood-Saxon single-particle functions spanning the 1s, 1p, and 2s-1d shells (ref. 9). No particular attempt was made to search for optimum values of α and β ; for a typical choice, the transition density $\rho_{\text{LSJ}}^{\text{if}}(r)$ and its truncated Gauss-Laguerre series representation shown in figure 1. (A larger number of terms is required than in the harmonic oscil-

lator case because the Wood-Saxon transition density falls off exponentially with distance, whereas the individual terms in the series representation have a Gaussian envelope.) The correspondence is quite good, except for the regions where the densities are very small.

REFERENCES

1. Haybron, R. M.; and McManus, H.: Excitation of Quadrupole and Octupole Levels of ^{12}C , ^{16}O , and ^{40}Ca by 156-MeV Protons. *Phys. Rev.*, vol. 140, no. 3B, Nov. 8, 1965, pp. 638-647.
2. Gillet, Vincent; and Melkanoff, Michel A.: Role of Particle-Hole Correlations in the Inelastic Scattering of Electrons from C^{12} , O^{16} , and Ca^{40} . *Phys. Rev.*, vol. 133, no. 5B, Mar. 9, 1964, pp. 1190-1199.
3. Glendenning, Norman K.: Coupled Channel Treatment of Inelastic Scattering Based on Microscopic Nuclear Descriptions. *Nucl. Phys.*, vol. A117, 1968, pp. 49-65.
4. Braley, Richard C.; and Ford, William F.: Inelastic Scattering Calculations with Projected Hartree-Fock Wave Functions. *Phys. Rev.*, vol. 182, no. 4, June 20, 1969, pp. 1174-1185.
5. Brink, D. M.; and Satchler, G. R.: *Angular Momentum*. Clarendon Press, Oxford, 1962.
6. Sawaguri, T.; and Tobocman, W.: Finite-Range Effects in Distorted-Wave Born-Approximation Calculations of Nucleon Transfer Reactions. *J. Math. Phys.*, vol. 8, no. 11, Nov. 1967, pp. 2223-2230.
7. Erdelyi, Arthur, ed.: *Higher Transcendental Functions*. Vols. 1 and 2. McGraw-Hill Book Co., Inc., 1953.
8. Glendenning, Norman K.; and Veneroni, Marcel: Inelastic Scattering Based on a Microscopic Description of Nuclei. *Phys. Rev.*, vol. 144, no. 3, Apr. 22, 1966, pp. 839-853.
9. Ford, William F.; and Braley, Richard C.: Hartree-Fock Calculations with Wood-Saxon Basis Functions. *Nucl. Phys.*, vol. A134, 1969, pp. 265-276.

TABLE I. - OVERLAP COEFFICIENTS^a FOR ELASTIC
AND INELASTIC TRANSITIONS IN ²⁰Ne

Elastic transition, 0 ⁺ → 0 ⁺		Inelastic transition, 0 ⁺ → 2 ⁺			
a, b	S _J (ii ab)	a, b	S _J (if ab)	a, b	S _J (if ab)
1, 1	1.93009	1, 3	-4.48480 (-2)	6, 10	6.74103 (-2)
1, 2	2.9913 (-1)	1, 4	8.53831 (-2)	7, 6	1.40121 (-2)
2, 2	7.01152 (-1)	2, 3	1.24356 (-1)	7, 8	5.23539 (-2)
3, 3	1.29565 (-1)	2, 4	-3.92796 (-1)	7, 9	8.93141 (-3)
4, 4	1.23920	3, 1	1.92589 (-2)	8, 5	-1.16449 (-2)
5, 5	1.95365	3, 2	-4.50232 (-2)	8, 6	1.56179 (-2)
5, 7	2.39522 (-1)	3, 3	-3.03809 (-2)	8, 7	-3.90190 (-3)
6, 6	3.83722	3, 4	-4.93584 (-2)	8, 8	7.07764 (-3)
6, 8	7.49017 (-1)	4, 1	3.83128 (-2)	8, 9	-6.94078 (-3)
7, 7	3.07065 (-2)	4, 2	-1.81644 (-1)	8, 10	1.13321 (-2)
8, 8	1.49829 (-1)	4, 3	6.20682 (-2)	9, 5	3.34721 (-2)
9, 9	1.83771 (-2)	4, 4	-3.10634 (-1)	9, 6	2.29125 (-2)
10, 10	1.02197 (-2)	5, 6	-3.03551 (-3)	9, 7	3.77817 (-3)
		5, 8	2.27451 (-2)	9, 8	4.12532 (-3)
		5, 9	7.96833 (-2)	9, 9	-4.24863 (-3)
		6, 5	1.62547 (-3)	9, 10	-1.02218 (-3)
		6, 6	-5.02013 (-3)	10, 6	3.46070 (-2)
		6, 7	-1.37811 (-2)	10, 8	6.02385 (-3)
		6, 8	2.18438 (-2)	10, 9	9.47013 (-4)
		6, 9	-3.85836 (-2)	10, 10	-2.59567 (-3)

^aThe single-particle states φ_a are labeled by $a = (1, \dots, 10)$
for $\varphi_a = (1s_{1/2}, 2s_{1/2}, 1d_{3/2}, 1d_{5/2}, 1p_{1/2}, 1p_{3/2},$
 $2p_{1/2}, 2p_{3/2}, 1f_{5/2}, 1f_{7/2})$.

^b $S_J(ii|ba) = S_J(ii|ab)$.

TABLE II. - DENSITY COEFFICIENTS ρ_{LSJn}

FOR ELASTIC AND INELASTIC

TRANSITIONS IN ^{20}Ne [Expansion parameters: $\alpha = 0.5593$;
 $\beta = 0.8 \text{ fm}^{-1}$.]

n	Elastic transition, $0^+ \rightarrow 0^+$	Inelastic transition, $0^+ \rightarrow 2^+$	
	Density coefficient		
	ρ_{000n}	ρ_{202n}	ρ_{212n}
0	5.3423 (-1)	5.1295 (-2)	-2.6324 (-3)
1	-2.2250 (-1)	-1.2736 (-1)	3.0126 (-3)
2	-5.2752 (-4)	-4.3476 (-3)	1.1925 (-4)
3	-4.6650 (-3)	6.6777 (-7)	-1.8232 (-8)
4	6.0398 (-7)	-4.4295 (-9)	2.5105 (-10)
5	1.0555 (-8)	5.4102 (-10)	4.5131 (-11)
6	4.7921 (-9)	6.8837 (-9)	-2.3466 (-10)
7	1.0035 (-11)	6.7184 (-9)	-3.2639 (-10)
8	-9.5549 (-10)	-1.0776 (-9)	-1.4097 (-10)
9	5.2544 (-11)	-9.5644 (-9)	1.4020 (-10)

TABLE III. - NUCLEAR MATTER RADIUS AND REDUCED

ELECTROMAGNETIC TRANSITION

PROBABILITY FOR ^{20}Ne

	Calculated	Experimental
Nuclear matter radius, r, fm	2.774	2.79
Reduced electromagnetic transition probability, B(E2), $e^2\text{fm}^4$	160.34	286.5

TABLE IV. - BORN APPROXIMATION ELECTRON
SCATTERING FORM FACTORS FOR ELASTIC
AND INELASTIC TRANSITIONS IN ^{20}Ne

Square of momentum transfer, q^2 , fm^{-2}	Elastic transition, $0^+ \rightarrow 0^+$	Inelastic transition, $0^+ \rightarrow 2^+$
	Form factor, $ F(q) ^2$	
0	1.0	0
0.5	2.6856 (-1)	6.4541 (-3)
1.0	6.5945 (-2)	6.8279 (-3)
1.5	1.3860 (-2)	3.5390 (-3)
2.0	2.1062 (-3)	1.1193 (-3)
2.5	6.2199 (-4)	1.5903 (-4)
3.0	3.1148 (-5)	2.0261 (-6)
3.5	1.3677 (-4)	9.0944 (-5)
4.0	1.6683 (-4)	1.7703 (-4)
4.5	1.4272 (-4)	2.0258 (-4)
5.0	1.0329 (-4)	1.8223 (-4)
5.5	6.7898 (-5)	1.4233 (-4)
6.0	4.1961 (-5)	1.0117 (-4)

TABLE V. - PROTON SCATTERING FORM
 FACTOR COEFFICIENTS f_{LSJN} FOR
 ELASTIC AND INELASTIC
 TRANSITIONS IN $^{20}\text{Ne}^a$

[Expansion parameters: $\alpha = 0.5593$;
 $\beta = 0.8 \text{ fm}^{-1}$.]

N	Elastic transition, $0^+ \rightarrow 0^+$	Inelastic transition, $0^+ \rightarrow 2^+$	
	Form factor coefficients		
	f_{000N}	f_{202N}	f_{212N}
0	-3.1382 (+3)	-9.0077 (+2)	-4.5644
1	1.0660 (+3)	5.8531 (+2)	2.2725
2	-8.6744 (+1)	2.5171 (+1)	1.1510 (-1)
3	2.7019 (+1)	1.4187 (-2)	4.0569 (-5)
4	-3.0411 (-3)	-2.6422 (-2)	-8.4441 (-5)
5	-7.7322 (-4)	2.4913 (-2)	7.7467 (-5)
6	4.1770 (-4)	-1.5616 (-2)	-4.6899 (-5)
7	-1.2930 (-4)	6.2597 (-3)	1.7943 (-5)
8	1.8187 (-5)	-1.4507 (-3)	-3.8944 (-6)
9	-7.0469 (-7)	1.4755 (-4)	3.6049 (-7)

^aSee text for details of the nucleon-nucleon interaction and its expansion.

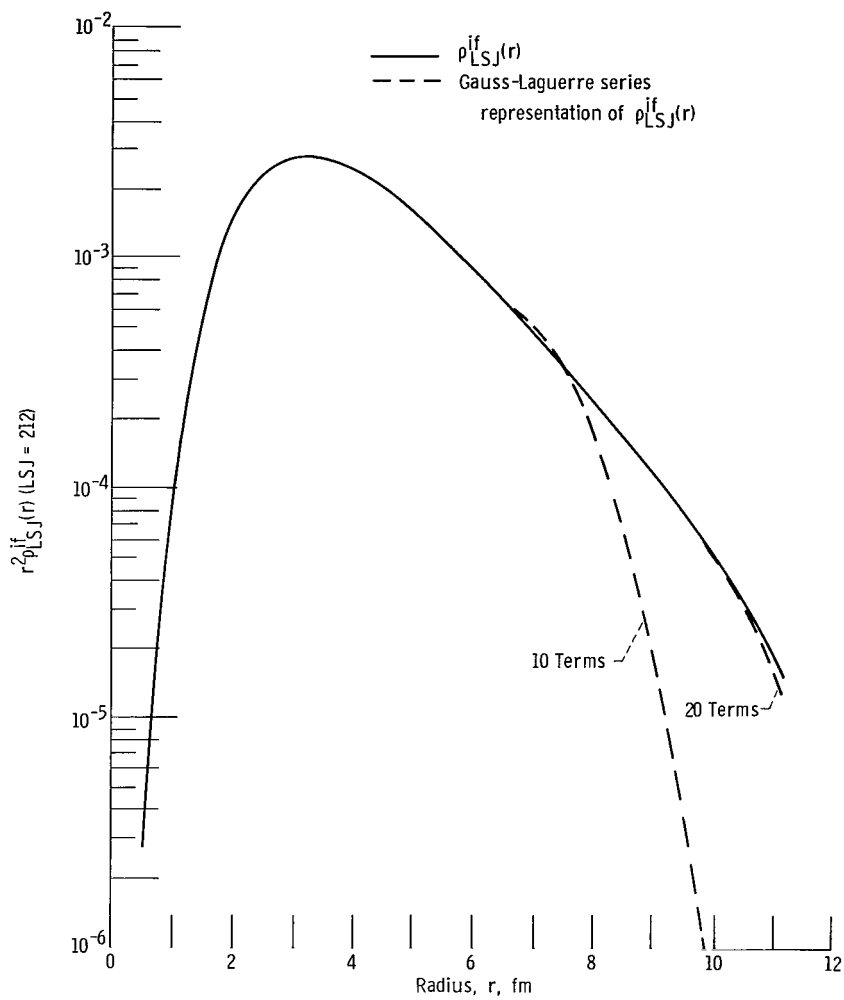


Figure 1. - Effect of truncation on Gauss-Laguerre series representation for a Wood-Saxon inelastic transition density $\rho_{LSJ}^{if}(r)$. Inelastic transition $0^+ \rightarrow 2^+$ for neon-20; expansion parameters: $\alpha = 0.5$; $\beta = 0.8 \text{ fm}^{-1}$.



10U 001 49 51 3DS 70185 00903
AIR FORCE WEAPONS LABORATORY /WLOL/
KIRTLAND AFB, NEW MEXICO 87117

ATT E. LOU BOWMAN, CHIEF, TECH. LIBRARY

POSTMASTER: If Undeliverable (Section 1
Postal Manual) Do Not Rc

"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."

— NATIONAL AERONAUTICS AND SPACE ACT OF 1958

NASA SCIENTIFIC AND TECHNICAL PUBLICATIONS

TECHNICAL REPORTS: Scientific and technical information considered important, complete, and a lasting contribution to existing knowledge.

TECHNICAL NOTES: Information less broad in scope but nevertheless of importance as a contribution to existing knowledge.

TECHNICAL MEMORANDUMS: Information receiving limited distribution because of preliminary data, security classification, or other reasons.

CONTRACTOR REPORTS: Scientific and technical information generated under a NASA contract or grant and considered an important contribution to existing knowledge.

TECHNICAL TRANSLATIONS: Information published in a foreign language considered to merit NASA distribution in English.

SPECIAL PUBLICATIONS: Information derived from or of value to NASA activities. Publications include conference proceedings, monographs, data compilations, handbooks, sourcebooks, and special bibliographies.

TECHNOLOGY UTILIZATION PUBLICATIONS: Information on technology used by NASA that may be of particular interest in commercial and other non-aerospace applications. Publications include Tech Briefs, Technology Utilization Reports and Notes, and Technology Surveys.

Details on the availability of these publications may be obtained from:

SCIENTIFIC AND TECHNICAL INFORMATION DIVISION
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Washington, D.C. 20546